

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.18e-01

Global applicability domain: Inside

Local applicability domain index: 5.00e-01

Confidence level: 6.78e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>HFC-41</div> <div>Measured: 0.51</div> <div>Predicted: 3.18e-01</div>	<div>Image not found</div> <div>Methyl formate</div> <div>Measured: 0.03</div> <div>Predicted: -0.0580</div>	<div>Image not found</div> <div>Methanol</div> <div>Measured: -0.770</div> <div>Predicted: -0.606</div>
<div>Image not found</div> <div>Methylamine</div> <div>Measured: -0.570</div> <div>Predicted: -0.633</div>	<div>Image not found</div> <div>Formaldehyde</div> <div>Measured: 0.35</div> <div>Predicted: 2.38e-01</div>	